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The University of Queensland Surat Deep Aquifer Appraisal Project (UQ-SDAAP)

Scoping study for material carbon abatement via carbon capture and storage

Supplementary Detailed Report

Sector model for carbon dioxide injection simulations – gridding and upscaling

30 April 2019

Research Team

Mr Iain Rodger, The University of Queensland
Mr Sebastian Gonzalez, The University of Queensland
Prof Jim Underschultz, The University of Queensland

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Referenced throughout the UQ-SDAAP reports as **Rodger et al. 2019e.**

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1. Executive summary

The UQ-SDAAP research program involved modelling at several scales, ranging from analytical single well models (e.g. for well test analysis) to limited area, 2-phase sector models (e.g. for testing sensitivity to geological concepts for the Transition Zone), to larger-scale, 2-phase models for wide-area injection simulation, to very large regional, single phase groundwater models. This report discusses gridding and upscaling for CO_2 injection simulation.

Sector and groundwater model grids (used as the basis for numerical simulations of CO_2 injection and groundwater flow) have been created, and populated with properties, based on the regional static model provided by the UQ-SDAAP geology, geophysics and petrophysics team.

Re-gridding of the regional static model was required to reduce the cell count (to make simulations less computationally expensive) and to remove some features of the grids that, while not a problem for a static geological model, would cause convergence issues for numerical simulations.

Modifications to the notional injection sector model grid were made to represent the boundary conditions at the top of the Ultimate Seal and bottom of Blocky Sandstone Reservoir.

A ‘pseudo boundary’ area was created in the Notional Injection Sector model to allow the effects of managed aquifer recharge (MAR) in the north of the Surat Basin to be included in the CO_2 injection models.

The resulting grids are considered a reasonable realisation of the structure and properties of the Blocky Sandstone Reservoir, Transition Zone, and Ultimate Seal that will capture all relevant features that may impact the dynamic simulation results.

2. Introduction

The purpose of this report is to capture how key models were gridded and upscaled in the project. It offers more detail and discussion than is found in the UQ-SDAAP, main project report (Garnett et al. 2019d).

The regional static model was created by the UQ-SDAAP geology, geophysics and petrophysics team for the purpose of regional-scale geological visualisation. This static model also served as a basis for running dynamic simulations that investigate notional large volume CO_2 injection and storage, including the interaction of this process with regional groundwater systems, and with other anthropogenic activities in the same geology. To accomplish this, the regional geological model needed to be modified for use in dynamic simulations representing various notional CO_2 injection scenarios. The modifications were intended to:

a. Reduce the number of cells to make the simulations less computationally expensive/time consuming, while still providing a reasonable representation of the fluid behaviour;

b. Remove gridding issues, which would cause convergence problems within the numerical simulations; and

c. Add cells to allow more reasonable representation of the fluid behaviour at boundaries of the model in the North (where MAR injection could have some influence) and on the top/bottom boundaries of the model.

This document outlines the modifications made, and provides a description of the resulting models that were subsequently used for the UQ-SDAAP dynamic modelling.

3. Clipping and upgridding to reduce cell count

The regional static geological model developed by the UQ-SDAAP geology, geophysics and petrophysics team is extremely detailed, with approximately 104 million cells over 47 layers between the top of the Ultimate Seal and bottom of the Blocky Sandstone Reservoir. It was necessary to reduce the number of cells for dynamic modelling to make the simulations less computationally expensive and able to run on the UQ-SDAAP software/hardware without convergence errors.

Two grids were created. One (the "Notional Injection Sector model grid") was used for multiphase models of notional CO_2 injection to be run in reservoir simulation software (CMG GEM) that considers all the complications of multiphase flow in regions around the notional CO_2 injection locations, where both formation water and CO_2 may occur over the time scale of the simulation. This grid only covered the geographic area around the notional injection sites (65 x 115 km). This reduced the cell count substantially compared to that in the geographic area of the regional static model. The cell count was further reduced by "upgridding" (re-gridding the model with larger cells) in parts of the model where high levels of detail in the static geological model occurred that were unnecessary for representing changes in fluid flow due to notional CO_2 injection.

A second grid (the "groundwater model grid") was used as an input for groundwater impact modelling. In this case the model is single phase and is primarily concerned with understanding the far field pressure transmission from notional large scale CO_2 injection. The groundwater model can also account for hydrodynamic boundary conditions including recharge and discharge. This grid covered was for the same subsurface volume as the regional static model, but with the cell count reduced by "upgridding".

This process of reducing the cell count involved three steps:

1. Clipping the regional static model to the area of interest (for the notional injection sector model only) – see section 3.1
2. Upgridding both models using larger cells. For the notional injection sector model, this was based on the principle of maintaining detail in areas where multiphase (i.e. CO_2 and water) flow was likely to occur, while coarsening cells in parts of the model where single phase (water only) flow was expected – see section 3.2
3. Upscaling the properties of the regional static model to the new larger grid cells, so the simulated behaviour of a dynamic model using the new grids, would replicate the behaviour of equivalent models using the original grid – see section 3.3

3.1 Notional injection sector model area

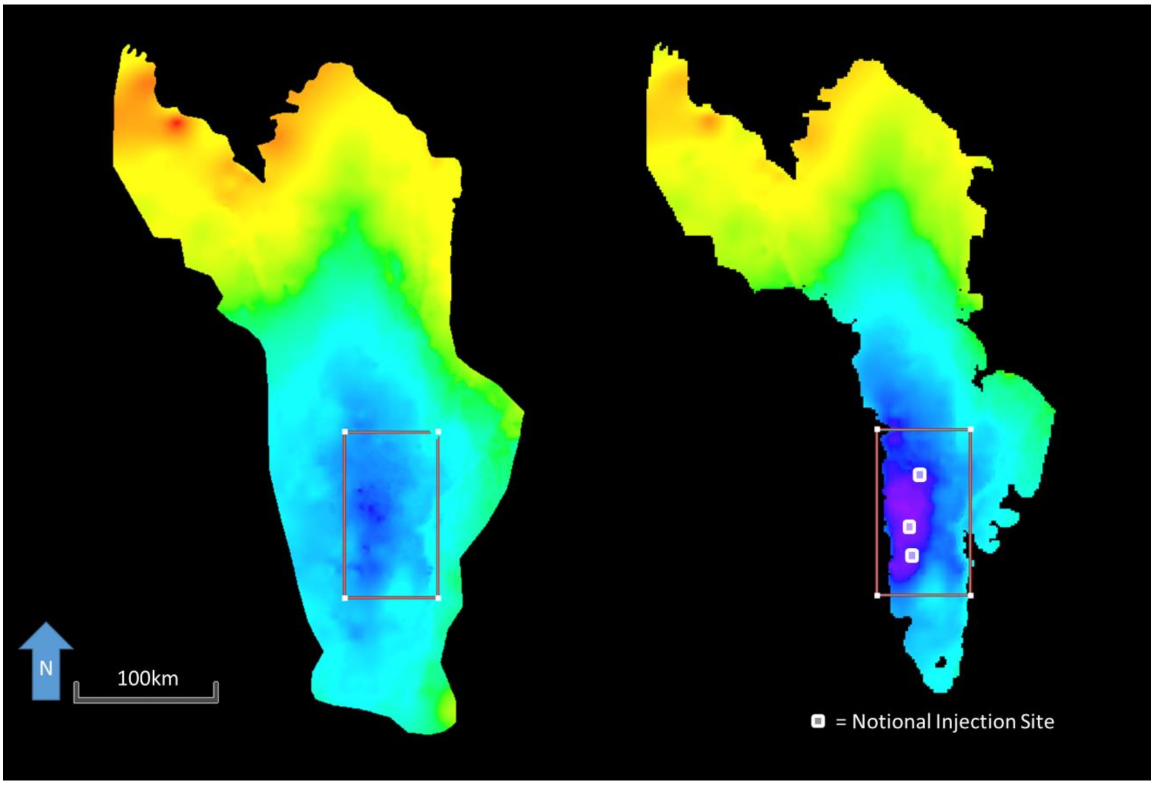
The UQ-SDAAP project determined the boundary for the Notional Injection Sector model based on the following criteria:

1. The notional injection sector model should include all notional injection sites (rather than modelling single injection locations in separate models) to allow for understanding any pressure interference between sites, and optimise injection rates between sites. This allows for several different roll-out scenarios to be tested (simulated) and more accurately represented. See Wolhuter et al. (2019a) for more information on the notional injection sites
2. the notional injection sector model should be large enough so that even in a credible worst-case scenario (i.e. most significant lateral migration of CO_2), the simulated CO_2 plume would not reach the edge of the model area
3. The western boundary of the notional injection sector model should occur further west than the 'pinch-out' of the Blocky Sandstone Reservoir. This would allow the effects of increased pressure build-up caused by the proximity of the 'pinch-out' to be modelled in a more reasonable fashion than if a boundary condition mimicking this effect had to be specified for the western boundary of the model

4. The eastern boundary should extend beyond the Moonie and Goondiwindi fault systems, thus including them in the model area. This would allow the pressure build-up at these faults to be simulated, and allow testing various fault sealing scenarios (sealing, partially sealing or not sealing) and its impact on injectivity and pressure build-up

Based on these criteria, the notional injection sector model was created in a 65km x115km area covering the deepest part of the Surat Basin, as shown in Figure 1

Figure 1 Location of the notional injection sector model (red box) relative to the top of the regional static model (left) and extent of Blocky Sandstone Reservoir (right). Colour indicates depth structure from sea level (blue/purple is deeper). Notional Injection Sites shown as white squares.



3.2 Upgridding

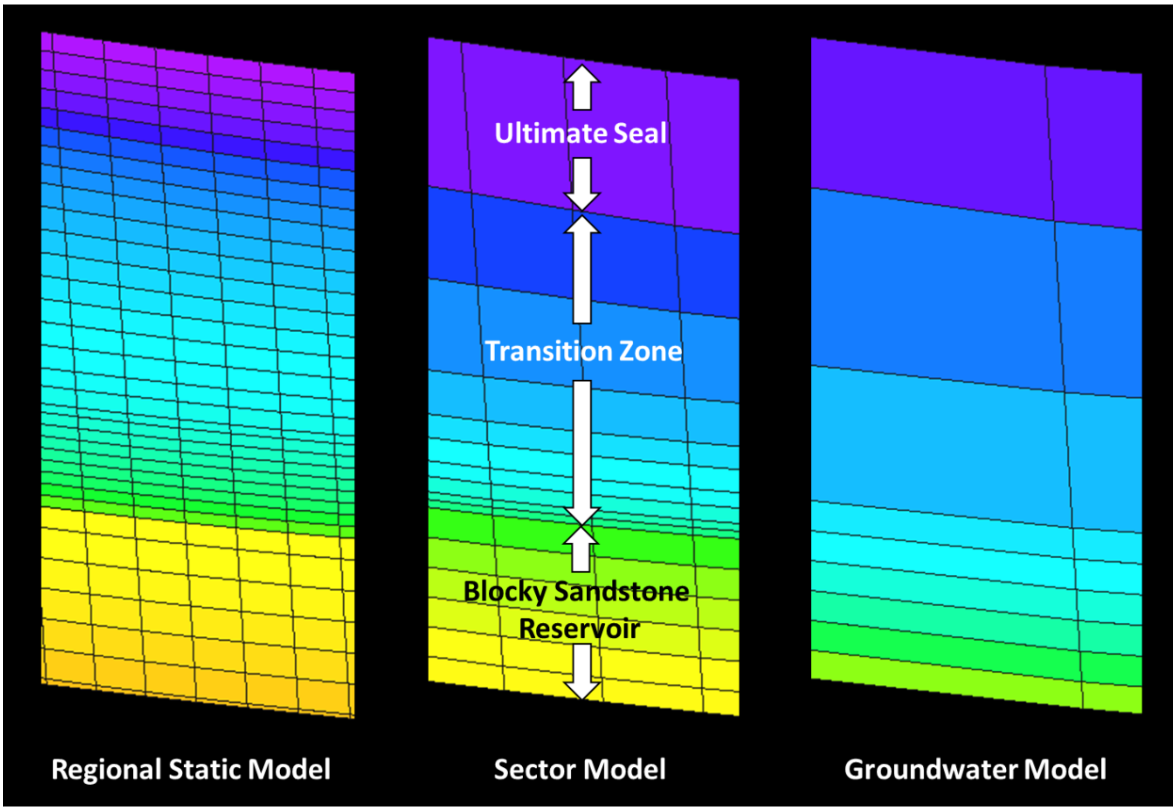
Reducing the area of the model from the entire Surat Basin to the notional injection sector reduced the cell count significantly from 104 million to 6 million cells, but the count could be reduced further by "upgridding" the model. This method was applied to both the notional injection sector model grid and the groundwater model grid, although the degree of the "upgridding" was slightly different in each case.

For the notional injection sector model, UQ-SDAAP re-gridded the model using 500m x 500m grid blocks, and reduced the number of layers, from 47 down to 19 (before the addition of layers to act as top and bottom boundaries, as described in section 5.2). The process for re-layering/re-gridding the model was performed in Petrel using the original surfaces/zones provided in the regional static model (Gonzalez et al. 2019b). Each zone was re-layered within the new 'empty' grid, which was then repopulated by upscaling the original model (see section 3.3). The re-layering process was different for each layer and for the two different models.

In the Transition Zone and Ultimate Seal it was determined that layers could be eliminated based on the results from smaller 10km x 10km notional injection sector models that were run to test the behaviour of fluids in the Transition Zone (Rodger et al. 2019c). These earlier simulations indicated that it was unlikely that any CO_2 would migrate further vertically than the lowest ~10m of the Transition Zone even for the most permeable and vertically connected geological scenarios in the sensitivity analysis. This meant the any flow above this point would likely be single phase (water only) and could still be represented accurately by larger cells as long as they were appropriately parameterised. For this reason, the new models had only one layer of cells representing the Ultimate Seal, when the regional static model had eight. Similarly, the 20 layers in the Transition Zone were replaced with nine layers for the notional injection sector model, and with only two layers for the Groundwater model. The notional injection model had layers with varying thickness in the Transition Zone, with thinner layers at the bottom where multiphase behaviour (such as capillary pressure, relative permeability and residual trapping) would be most important. This was implemented to accurately capture multiphase flow behaviour in this region of the model.

The layers in the Blocky Sandstone Reservoir remained almost the same as in the regional static model (aside from the minor adjustments described in Section 4) and in places where the reservoir is thinner there can be fewer than 19 layers cells as the lower layers ‘pinch-out’. A comparison of this layering scheme in the final Notional Injection Sector model with the original scheme in the regional static model is shown in Figure 2.

Figure 2 A comparison of the gridding in the three models (regional static model, notional injection sector model, and groundwater model). Note the thinner layers at the lowest part of the Transition Zone in the notional injection model. In some geographic locations there may be more layers present than are shown in this figure, depending on the thickness of the Blocky Sandstone Reservoir.



The groundwater model grid was modified in a similar fashion to the Notional Injection Sector model, but using larger grid blocks (1500m x1500m) to approximately coincide with the grid used in the Office of Groundwater Impact Assessment (OGIA) groundwater model of the Surat Basin (OGIA 2016). Coarser layering was used throughout the transition zone in the groundwater model grid (as multiphase behaviour was not a concern), resulting in a total of 14 layers across the Blocky Sandstone Reservoir, Transition Zone and Ultimate Seal. Similar to the notional injection sector mode, all 14 layers were not necessarily present everywhere in the model. The number of layers was dependent on the total thickness of the Blocky Sandstone Reservoir at any location. An example section of the new grid is shown in Figure 2.

3.3 Upscaling of properties

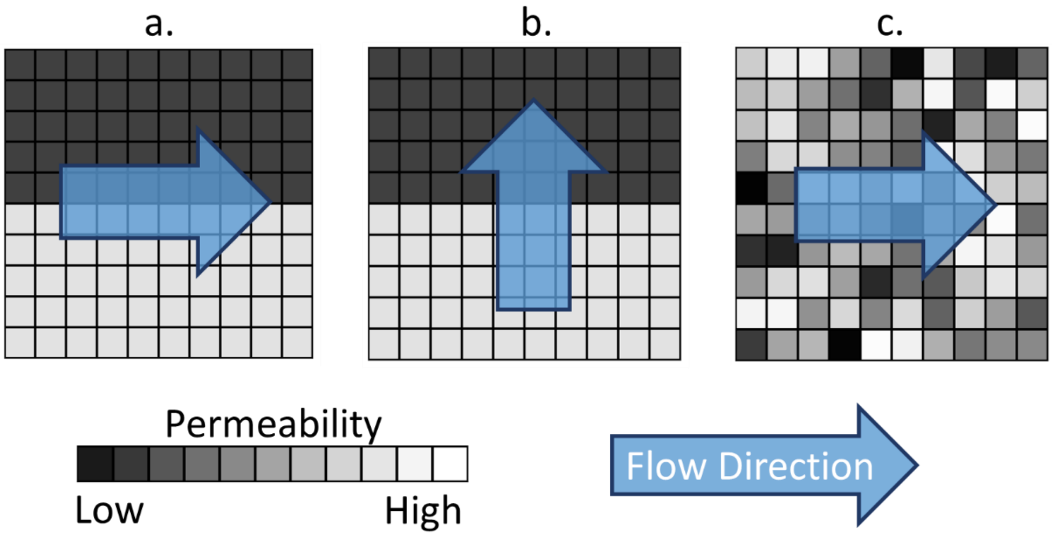
After creating the new coarser grids through “upgridding” it was then necessary to populate them with properties. In this case the properties required were effective porosity, and horizontal and vertical permeability. These had been defined in the regional static model by the UQ-SDAAP geology, geophysics and petrophysics team (Gonzalez et al. 2019b). The notional injection sector model and groundwater model grids were populated by upscaling the properties from the regional static model to these new coarser grids.

The UQ-SDAAP project used two different upscaling methods; volume weighted arithmetic averaging for effective porosity, and Petrel’s ‘flow-based upscaling’ for permeability (horizontal and vertical). The same methods were used to populate the notional injection sector model grid and groundwater model grid.

Volume weighted arithmetic averaging for effective porosity upscaling was chosen as a standard method, which would retain the overall pore volume present in the same volume of the regional model (as porosity is a volumetric/ additive property) (Cannon 2018). This meant the upscaling process did not alter the average porosity for cells in the models, but did narrow the distribution of porosities due to the larger cell sizes in the upgridded models.

There are many difficulties associated with appropriately upscaling permeability (which relate to scale, direction, and geometry dependence due to things such as in situ stress) for use in dynamic models. In different situations the arithmetic, geometric, or harmonic averages could be more appropriate. To demonstrate this issue, three hypothetical permeability upscaling scenarios are shown in Figure 3.

Figure 3 Three hypothetical permeability upscaling scenarios: (A) represents flow parallel to high and low permeability layers, (B) is flow perpendicular to the same layered system, and (C) is flow through a random field. All have the same arithmetic average permeability.



These three grids have the same arithmetic average permeability, but the flow behaviour in the direction shown in each would be very different. If the flow is parallel to layering (as in Figure 3 A) the overall flow will be a combination of the flow through the high and low permeability layers. The low permeability layer will have less flow, but will not significantly impact the flow through the higher permeability parts (as they would in Figure 3 B – see following paragraph). If the dark cells had zero permeability (and thus no flow), the effect would be to half the cross sectional area for flow, equivalent to halving the permeability of the larger block. In this case, the thickness weighted arithmetic average would usually be considered an appropriate upscaling method (Cannon 2018).

In contrast to this, flow perpendicular to permeability ‘layers’[1] (as shown in Figure 3 B) would be significantly reduced by the lower permeability in the upper layer, and the overall bulk permeability of the larger block would thus be much lower than the bulk permeability in Figure 3 A. In the specific case where the dark cells in Figure 3 B had zero permeability, the overall permeability in the direction of flow shown would be zero as the dark cells would prevent any flow. The Harmonic average could be used in this case, and is often used for upscaling of vertical permeability (Cannon 2018).

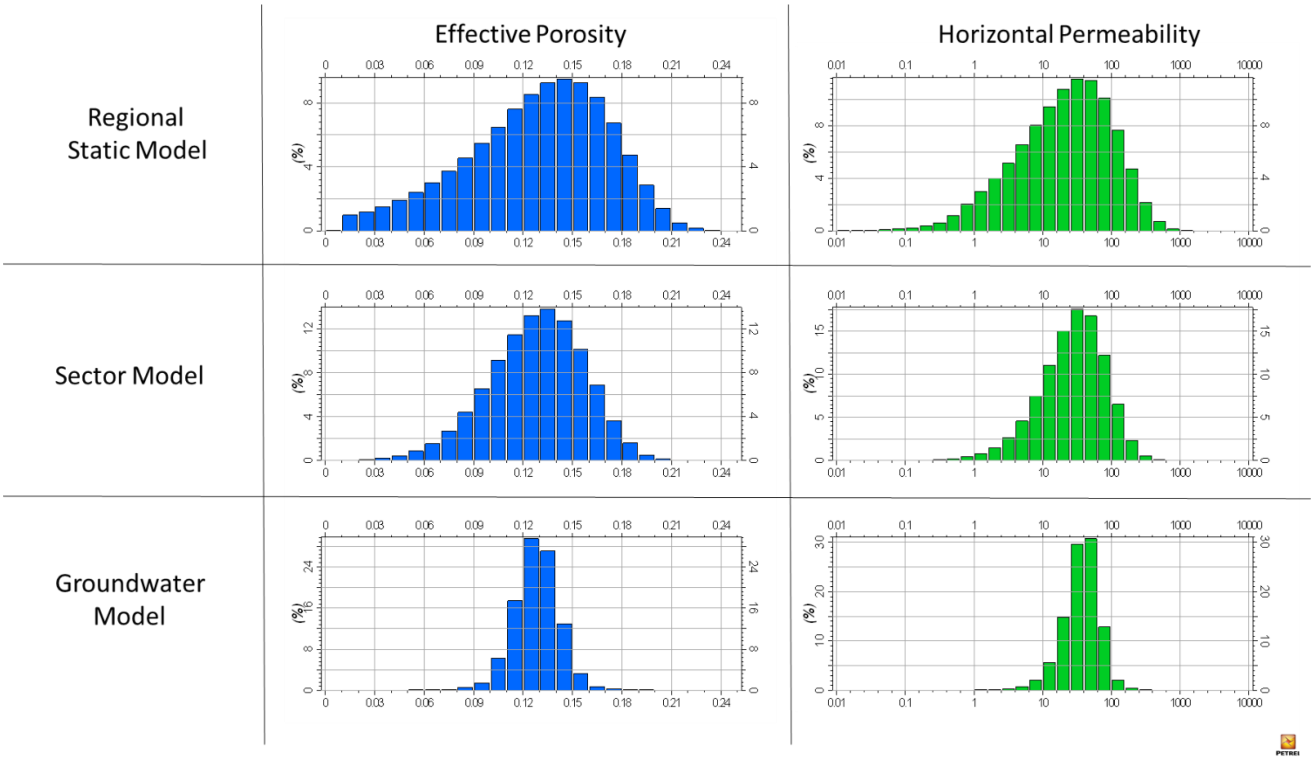
Permeability upscaling for very disordered fields (e.g. Figure 3 C) is even more challenging. Neither the arithmetic, nor harmonic average would accurately represent the complex flow through such a block. The geometric average is sometimes used for permeability upscaling in these cases, but low values have been found to cause issues when using this method (Jensen 1991).

The ‘Flow-based upscaling’ option built in to Schlumberger’s Petrel software was used to upscale the properties in the UQ-SDAAP models to avoid these issues. ‘Flow-based upscaling’ is a numerical (rather than statistical) upscaling method, where the finite difference method is used to simulate the flow across each cell in the new grid, using the combination of grid blocks in the regional scale model which would be within that individual cell in the new grid (Cannon 2018). After calculating the flow, the permeability of the new grid cell is determined, which would be associated with the calculated flow behaviour. This method is slightly more time-consuming than other averaging methods for permeability, but avoids the issue of ‘choosing’ the appropriate average to use for upscaling. The calculated permeability for the cells should result in numerical simulations that produce results that are similar to those that would be obtained using the original grid, particularly if the flow is single phase (water) only.

To sense check the effects of this upscaling on the properties, UQ-SDAAP created histograms of the properties in the notional injection sector model area (i.e. equivalent ‘volumes’) for all three grids. An example comparison for the effective porosity and (mid-case) horizontal permeability in the Blocky Sandstone Reservoir is shown in Figure 4. This demonstrates that upscaling the properties reduces the spread (or variance) of the data for both properties, dependant on the scale of the new grid relative to the old one. There is a more significant difference between the groundwater model and regional model due to the larger grid size used in the groundwater model. Importantly, the mean value for porosity remains the same for all models.

[1] The term layers is used here, but the same would apply in the scenario where the high and low permeability streaks were ‘layered’ laterally (in the x or y directions), equivalent to rotating the field in **Error! Reference source not found.** rather than rotating the flow direction.

Figure 4 *Comparison of grid properties of the Blocky Sandstone Reservoir in the three models. Permeability shown here is the mid-case from petrophysics (Harfoush et al. 2019c).*



The variance of the permeability is also reduced by the upscaling process, again more significantly for the groundwater model. The *arithmetic* mean permeability of cells is also reduced (by approximately 1.5mD for the groundwater model). This is likely due to low permeability cells limiting flow, even if the other cells which contribute to the new larger cell have significantly higher permeability (and is why the arithmetic average is not always suitable for permeability upscaling).

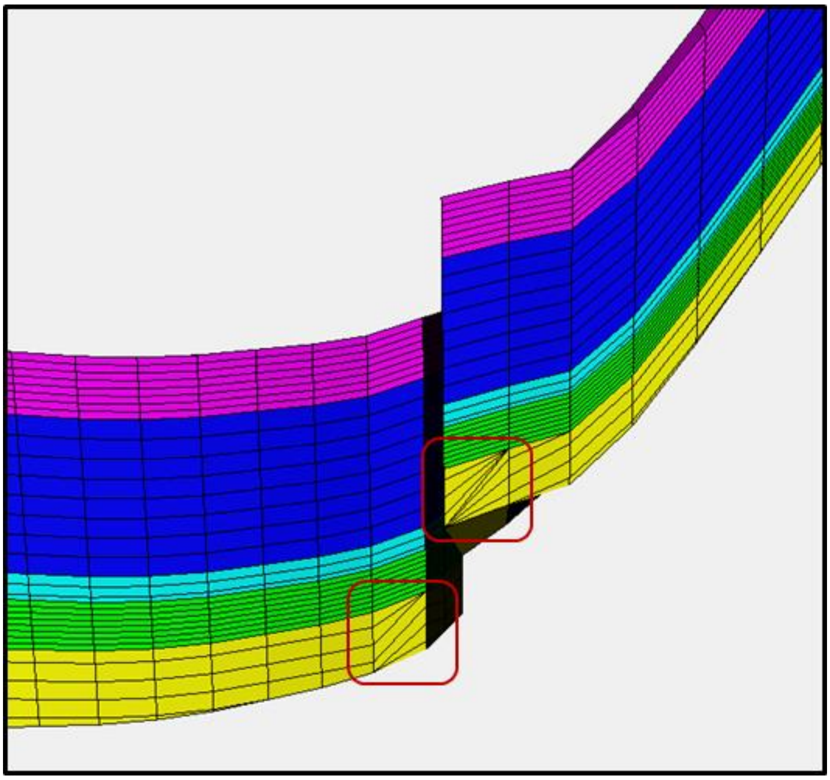
Appropriate well or laboratory testing (core, wireline and dynamic/flow testing) of appraisal wells in the notional injection site area would be required to improve the understanding of the porosity and permeability of the Blocky Sandstone Reservoir on all scales, and would seem necessary to allow more accurate modelling of CO_2 injection into the Blocky Sandstone Reservoir in the deepest parts of the Surat Basin.

4. Adjustment of gridding near faults

The regional static geological model used a corner-point grid, where the position and geometry of every grid block is defined by the location (x,y,z) of all eight corners of the block. This choice of gridding is useful as it allows cells to more accurately replicate the structure of the 'real' geology, in particular around faults. This is especially relevant for the UQ-SDAAP dynamic models where buoyancy (i.e. dip of layering) is important, or where discontinuities of layering is significant near fault zones.

The regional static geological model had several cell geometries, particularly around faults, that could cause convergence issues for dynamic numerical simulations. An example of this is shown in Figure 5 where cells are extremely distorted around the faults, with many cells in the Blocky Sandstone Reservoir "pinching out" (i.e. reaching zero thickness) in multiple dimensions. It was therefore necessary to re-grid the model in certain locations to avoid these problems.

Figure 5 *An example of gridding in the regional geological static model that could cause convergence issues in dynamic model simulations. The yellow cells near the fault (black) indicated in the red boxes have become extremely distorted, with multiple cells "pinching out" in all directions.*



While re-gridding, a number of other adjustments were made (discussed in more detail later in this report), but the two changes to the gridding process (performed in Petrel) that were specifically intended to prevent these cell geometries were:

1. Using 'zig-zag' vertical faults
2. Using the top of the 'zone' in the model, rather than the original surface, as the reference for layering the model in the Blocky Sandstone Reservoir

Using 'zig-zag' faults means the faults are modelled along the edges of grid blocks they pass through. They will thus appear to 'zig-zag' along the *i* and *j* (x and y) edges of these cells in the resulting grid, which will reduce the deformation of the cells around the fault. Vertical faults were also used, so any fault in the model had no dip associated with it and simply allows cells from the same layer on either side to be vertically offset from one another. This again reduces the deformation of the cells around the fault.

While reducing the deformation complexity of the faults, this method allowed us to retain the cross fault connections between different layers caused by the fault offset. UQ-SDAAP considered this to be the primary concern of the modelling around the faults, as any connections between the Blocky Sandstone Reservoir and shallower permeable layers could result in across fault flow of fluids into these shallower layers or causing increased pressure in shallower layers in excess of what would be expected if the faults did not exist.

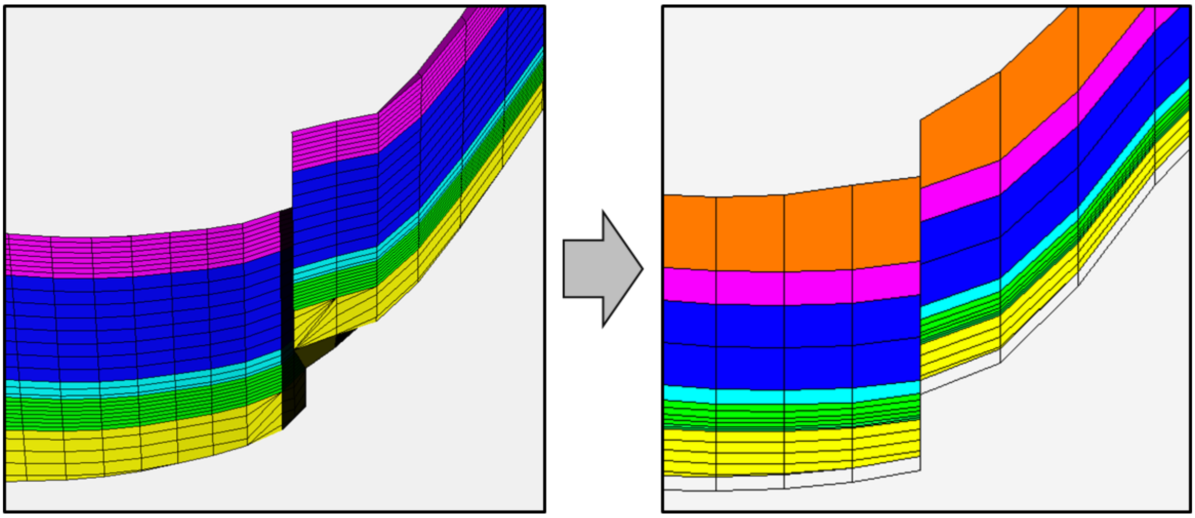
The disadvantage of using 'zig-zag' vertical faults is that they do not accurately represent fault geometries. This was unlikely to be a significant issue in the UQ-SDAAP models as the faults are relatively far from the notional injection sites, and CO_2 is very unlikely to reach them. This means the lack of dip is less significant, as the flow across any fault would be single phase (water) only. Thus, there is no buoyancy effect to drive vertical flow across/along an angled fault.

There remains some uncertainty in the existence, position and geometry of faults due to the relatively sparse seismic data available in the area of interest. If newly acquired or reprocessed/reinterpreted seismic indicated faulting occurred near the notional injection sites, these faults would need to be modelled in much greater detail than was possible in the UQ-SDAAP work scope.

When re-gridding the model, the layering in the Blocky Sandstone Reservoir was changed from following the original 'Top Blocky Sandstone' ***surface*** (which had been used to build the regional geological model) to instead following the top of the Blocky Sandstone Reservoir ***zone*** in the model. The difference between these two methods is subtle, but is very important around the faults. In the geological model, the Blocky Sandstone Reservoir and other zones are discontinuous in places; that is, there can be step changes in the depth of the top and bottom of the zones caused by faults. The original surfaces, which were based on seismic surfaces tied to well tops, do not feature these discontinuities, and are 'smoothed' across faults. This leads to gridding issues near the faults where the difference between the top of the zone and the original surface can be slightly different.

The results of these changes (as well as those described in sections 3.2 and 5.2) are shown in Figure 6.

Figure 6 The regional static geological model grid around a fault (left) and the re-gridded Notional Injection Model in the same area (right). The colours represent equivalent zones in each model: Yellow = Blocky Sandstone Reservoir, Blue-Green = Transition Zone, Pink = Ultimate Seal. Note that the image on the right shows the gridding after the additional changes described in the other sections of this report, hence the additional orange and white layers (section 5.2), and differences in layer count in each zone (section 3.2) are also shown here.



5. Notional injection sector grid modifications to represent boundary conditions

5.1 South, east and west boundaries

The boundary conditions used for the notional injection sector model were, for the most part, relatively straightforward for the south, east and west. These boundaries were defined as a number of 'leaky' (i.e. they would allow flow out of the model and into an assumed "aquifer" external to the model domain) using analytic (Carter-Tracy) aquifers within CMG GEM functionality (CMG 2018). This method makes use of dimensionless pressure and time terms to calculate the flow between the blocks at the edge of the reservoir model and the external 'aquifer' (Carter & Tracy 1960).

The defined external aquifers were connected to different zones within the model and had properties dependent on the zone they were connected to. For example, a 'Blocky Sandstone Reservoir' aquifer would be represented as having higher permeability than a "Transition Zone" aquifer.

5.2 Top and bottom boundaries

To represent the boundary behaviour at the top (above the Ultimate Seal and bottom (below the Base Surat Unconformity) of the model, UQ-SDAAP added two layers. The top layer (orange in Figure 6) is a relatively thick (100m), porous (20%) and permeable (100mD) layer that sits directly on top of the Ultimate Seal. This layer represents the Hutton Sandstone aquifer, which sits directly above the Ultimate Seal. The properties and geometry of this layer may not be accurate for the Hutton Sandstone, but the layer was not intended to accurately represent the Hutton. Instead it was intended to allow flow of fluids, or transmission of pressure, which would be limited mainly by the extremely low permeability of the Ultimate Seal (and not by the permeability of the Hutton). This layer was added because a closed boundary (no-flow) boundary above the Ultimate Seal would be unrealistic, and the added layer would allow assessment of (approximately) the volumes of fluid that could move from the Ultimate Seal into the Hutton Sandstone as a result of CO_2 injection.

The UQ-SDAAP project also added a layer at the bottom of the model (white in Figure 6). This layer is 20m thick and has properties that were varied to allow scenario testing to represent any flow that might occur into, or along, the Base Surat Unconformity surface itself at the base of the Blocky Sandstone Reservoir (whether due to weathering below the unconformity, or permeable sub-cropping porous formations). This is a more realistic representation of the lower boundary of the Blocky Sandstone Reservoir than a simple closed boundary condition. In particular, the addition of this layer allowed for testing the impacts of a 'leaky' Blocky Sandstone Reservoir pinch out, where flow could occur along the unconformity, potentially creating a connection between the Blocky Sandstone Reservoir and other stratigraphically higher sands in the Transition Zone as they sequentially pinch out against the Base Surat Unconformity surface towards the west.

5.3 Northern boundary

The final modification to the notional injection sector model grid was required to represent the managed aquifer recharge (MAR) injection occurring in the northern parts of the Surat Basin into the Blocky Sandstone Reservoir. This injection increases the pressure the Blocky Sandstone Reservoir in the north part of the basin, and could impact on the injectivity in the notional injection sites locations in the south part of the basin. While dynamic modelling suggests that this effect would be relatively small, based on current MAR volumes, UQ-SDAAP still considered it appropriate to create a boundary condition in the north that would allow us to represent the MAR injection under various future scenarios at different volumes.

To achieve this, a 'pseudo-boundary' was created by stretching the second, third and fourth last rows of cells at the far north of the notional injection sector model so their total combined length (N-S) was approximately 100km (Figure 7). This was intended to represent the volume of rock and fluid between the MAR injection location and the north of the UQ-SDAAP notional injection sector model. A very high permeability (4 Darcies) analytic aquifer was defined as the northern boundary condition for these cells to represent the extensive high permeability aquifer equivalent to the Blocky Sandstone Reservoir which exists in the northern depositional centre of the Surat Basin (Hayes et al. 2019a).

After stretching the grid, a single well was placed in the final row of cells and was used to control injection of water into the Blocky Sandstone Reservoir at rates based on the MAR injection to date. The parameters (including porosity, permeability and volume modifiers) of these 'stretched' cells were manually adjusted until the pressure response in these cells was similar to that predicted by groundwater models of MAR injection to date (Hayes et al. 2019a). The resulting horizontal permeabilities for the Blocky Sandstone Reservoir in the notional injection sector model 'pseudo-boundary' area are shown in Figure 8.

While the stretched cells do not accurately represent the geometry or properties of the Surat Basin and Blocky Sandstone Reservoir in the area north of the Notional Injection Sector mode, they should act as a reasonable 'pseudo-boundary' that mimics and equivalent of the MAR injection in the UQ-SDAAP Notional Injection Sector models. In the forward models of CO_2 injection, the 'MAR' well at the north of the pseudo-boundary area will inject water until 2054 at the estimated rates for the MAR scheme per OGIA (OGIA 2016).

The 'pseudo-boundary' cells will not be shown in the subsequent results of dynamic simulations.

Figure 7 The scale of the 'Pseudo- Boundary' area created by stretching 3 rows of cells in the notional injection sector model, shown overlain on the horizontal permeability distribution used in the groundwater model grid. The difference in permeability between the north and south parts of the groundwater model is due to two depo centres that are hypothesised by the UQ-SDAAP team. (Hayes et al. 2019a; Gonzalez et al. 2019b).

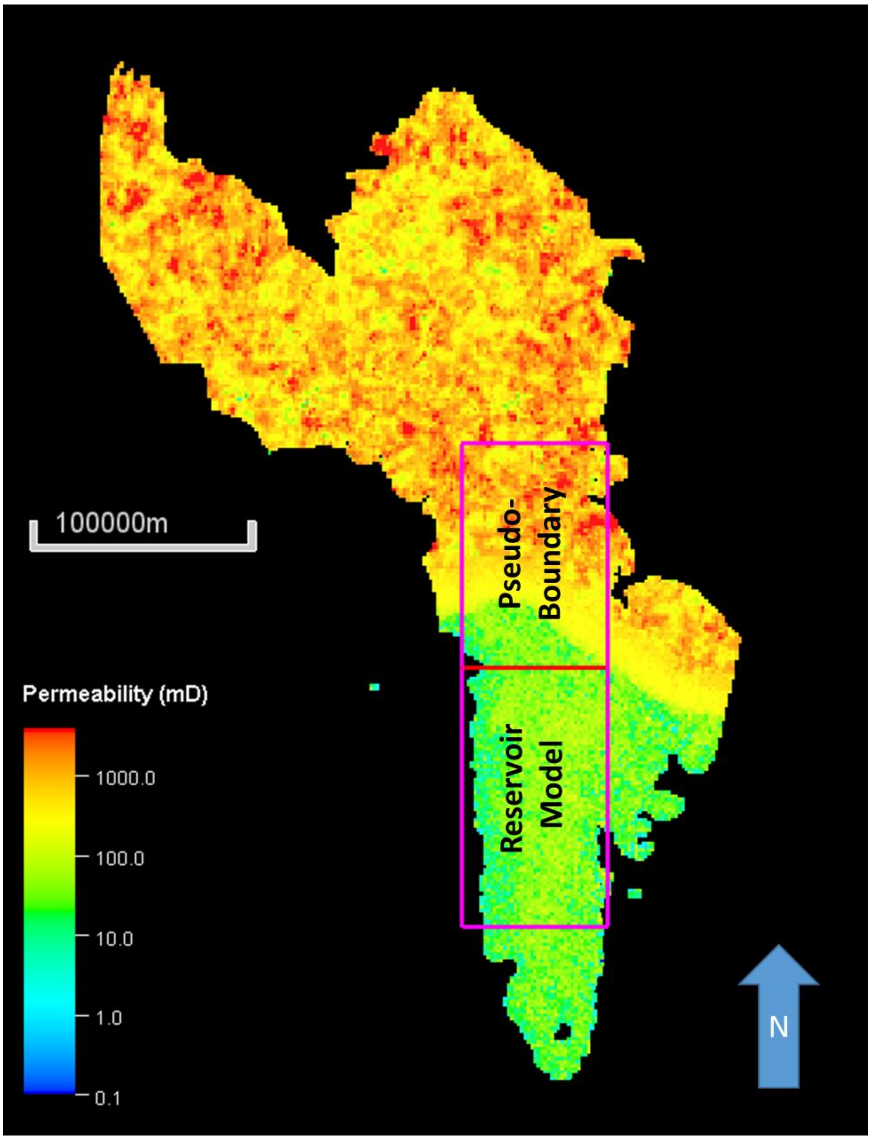
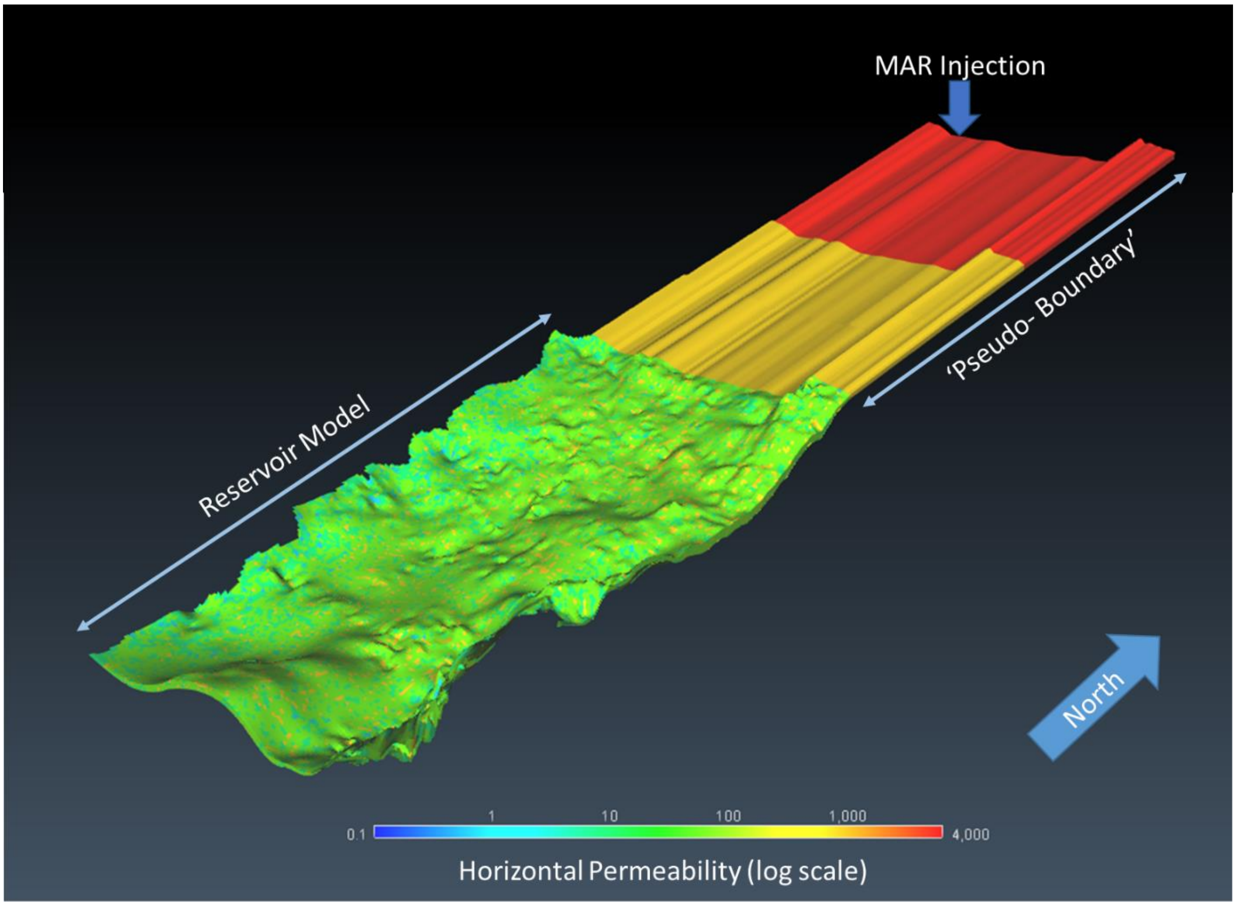


Figure 8 The structure and horizontal permeability of the Blocky Sandstone Reservoir in the notional injection sector reservoir model and 'pseudo-boundary'. Note that the permeability in the 'pseudo boundary' has similar trend to the groundwater model grid shown in Figure 7.



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